

Propanoic acid, 2-(1-oxopropoxy)-, methyl ester

61402-72-0 | DTXSID30485366

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.14

Global applicability domain: Inside

Local applicability domain index: 9.83e-01

Confidence level: 7.89e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Cumene</div> <div>Measured: 3.98</div> <div>Predicted: 3.95</div>	<div>Image not found</div> <div>Benzonitrile</div> <div>Measured: 4.46</div> <div>Predicted: 3.95</div>	<div>Image not found</div> <div>Nonene</div> <div>Measured: 3.83</div> <div>Predicted: 3.95</div>
<div>Image not found</div> <div>Butyl ether</div> <div>Measured: 3.89</div> <div>Predicted: 3.93</div>	<div>Image not found</div> <div>Hexyl acetate</div> <div>Measured: 4.58</div> <div>Predicted: 4.51</div>	